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NUMERICAL CONVERGENCE OF GYROKINETIC SIMULATIONS OF ION-TEMPERATURE-GRADIENT TURBULENCE

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We examine the convergence of particle-based nonlinear "gyrokinetic simulations" of ion-temperature-gradient (ITG) turbulence [1] with respect to numerical parameters. Our main focus is on convergence with respect to particle number, both through direct particle number scans and through "scrambling tests" that determine the relative effect of the noise due to particle discreteness. Results will also presented on convergence with respect to spatial resolution and system size.

This topic is of current interest in the modeling of fusion plasmas. Predictions that the proposed ITER tokamak reactor will not reach ignition [2] have been made on the basis of the IFS-PPPL model [3], underlying which is a database of nonlinear gyrofluid simulation results. Direct nonlinear gyrokinetic simulation provides a means to test the first-principles basis of the gyrofluid simulations and, thereby, of the IFS-PPPL model. For the "Cyclone DIII-D base case" described below, it has been found that gyrofluid simulations give a value of the thermal diffusivity χ_i roughly a factor of 3 higher than the gyrokinetic simulations, with larger differences if the temperature gradient is reduced [4]. These differences have a significant impact on predictions of ITER performance. It is therefore of great importance and interest to assess, and if possible establish, the validity of the gyrokinetic results.

The development of several advanced numerical algorithms, namely δf methods, flux-tube geometries, and quasiballooning representations, along with rapid increases in computer power have greatly increased the applicability and solidity of gyrokinetic simulations for fusion relevant plasma conditions. Even with the combination of these advances, however, truly convincing demonstrations of convergence with respect to the relevant numerical parameters provide challenges.

We focus on the Cyclone DIII-D base case parameter set which represents local parameters from an ITER-relevant DIII-D shot #81499, at $t = 4000$ms., and $r/a = 0.5$. A concentric-circular-cross-section model equilibrium is used, with $n_i = n_e$ and $T_e = T_i$. Additional simplifications in the simulation are (1) it is electrostatic, (2) the electrons are taken to be adiabatic, and (3) a single dynamical ion species (which represents the "bulk" ions) is used. These simplifications match those in the nonlinear gyrofluid simulations that underly the IFS-PPPL model. The simulation box size used is $125.7\rho_i$ (where ρ_i is the ion Larmor radius) in the perpendicular directions and one poloidal circuit in the parallel direction. The perpendicular mesh size is $0.9817\rho_i$, and 32 parallel grid cells were used.

Figure 1 (a) and (b) show respectively χ_i vs. time and the volume averaged ϕ^2 vs. time, where ϕ is the electrostatic potential, from a particle number scan.

The normalizations used are: efluxi = $\chi_{\rm i}L_{\rm ni}/(\rho_i^2 v_{\rm ti})$, and Time = $(tv_{\rm ti})/L_{\rm Ti}$, and els = $(1/N_{\rm g})\sum_g[(L_{\rm ne}/\rho_i)(e\phi(\boldsymbol{x}_g)/T_{\rm i})]^2$, where the sum is over 3D grid-cell index vectors $g = (i,j,k)$ and $N_{\rm g}$ is the number of grid cells. The simulations are for different numbers of particles: 0.5M, 1M, 2M, 4M, 8M, 16M, and 32M (where M$\equiv 10^6$). The curves are difficult to distinquish in black and white, but we can describe the trends. For 1M to 32M particles, there does not appear to be any systematic monotonic trend in $\chi_{\rm i}$ vs. particle number, except for some increase in the initial peak. (This increase is due to the fact that for larger particle number, the initial seed noise level is lower, so that the system must undergo a longer linear phase before saturation. This results in a more coherent state right before saturation, so that the saturation occurs at larger amplitude.) The 0.5M case shows secular growth in $\chi_{\rm i}$ beyond Time = 700. This is probably due to a noise-driven runaway process where in which the detailed entropy, most of which is due to noise, increases with the time integral of $\chi_{\rm i}$. The noise causes thermal transport ($\chi_{\rm i}$), both of which increase together. For 2M to 16M particles there is not a clear systematic trend in els. The mean value and relative oscillation amplitude increase for the lowest particle numbers, and the onset of the large fluctuations is earliest in the 0.5M case. The 32M case has the smallest relative oscillation amplitude. Separate diagnostics of the shearing rate and of the modal content of ϕ indicate that els is dominated by long wavelength modes whose relative contribution to the shearing rate is small. The variation in els appears to be a function primarily of detailed initial conditions more than of the particle number, and is not accompanied by a corresponding variation in $\chi_{\rm i}$. Detailed diagnostics of the dependence of the shearing rate on particle number will be shown. The primary conclusion is that $\chi_{\rm i}$ appears to be converged wrt. particle number.

In order to assess the impact of particle discreteness in more detail, the following scrambling test [5] of the noise level was performed. The gyrokinetic code was run saving restart files at selected times. New restart files were formed from these by scrambling the particle weight list. The gyrokinetic code was restarted from these scrambled restart files. The scrambling of the weights eliminates the physical turbulent fluctuations, but leaves a random fluctuation component which gives a measure of the noise due to particle discreteness. The restarted simulations were run long enough for stable geodesic acoustic fluctuations, which are present immediately after the scrambling, to damp. The resulting electrostatic potentials (or the shearing rates derived from it) are then characteristic of the noise inherent in the gyrokinetic simulation just prior to the scrambling. After the restart, the temperature gradient (only) was reduced to slightly below the linear marginally stable value in order to eliminate unstable ITG modes. The test was done using 8M particles in the simulation.

Shown in Figure 2 are the time histories of $\chi_{\rm i}$ and the mean squared $\boldsymbol{E}\times\boldsymbol{B}$ shearing rate $(L_{\rm Ti}S/v_{\rm ti})^2$ associated with the flux-surface-averaged electrostatic potential, both in the absence of scrambling and when the scrambling and gradient reduction is done at three times during the run. Both of these quantities are reduced after the scrambling. The relative reduction is less the later the scrambling is done, indicating a gradual buildup of noise. However, even at the latest time, the post scrambling values are down by an order of magnitude. This indicates that the relative impact of noise is small (or at most moderate at the latest time), and supports the conclusion that the simulations are converged with respect to particle number.

Thus, for robustly (linearly and nonlinearly) unstable situations such as the Cyclone DIII-D base case, numerical convergence is achieved with 2–4 particles per cell in our code.

We have observed an exception to this. Some parameter sets result in moderate linear instability and subsequent nonlinear evolution into stable states which have radially dependent flux-surface-averaged temperature gradients and $\boldsymbol{E} \times \boldsymbol{B}$ flows. In these situations the radial particle thermal flux asymptotes to zero. As many as 64 particles per cell are needed to observe this, since the stable nonlinear states become quite delicate as a threshold value (larger than the linear critical value) of the volume averaged temperature gradient is approached from below.

We have also undertaken simulations that demonstrate convergence with respect to parallel and perpendicular system size and with respect to parallel and perpendicular spatial resolution for robustly unstable cases. The results, which will be shown, demonstrate that the values typically used in our simulations are adequate for numerical convergence. Further system size and resolution tests are being undertaken for cases that yield nonlinearly stable states.

Acknowledgments

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[5] The scrambling noise test was proposed originally by M. Kotschenreuther, and valuable variations and refinements were suggested by W. Dorland and G.W. Hammett in private communications dating between 1995 and 1997.

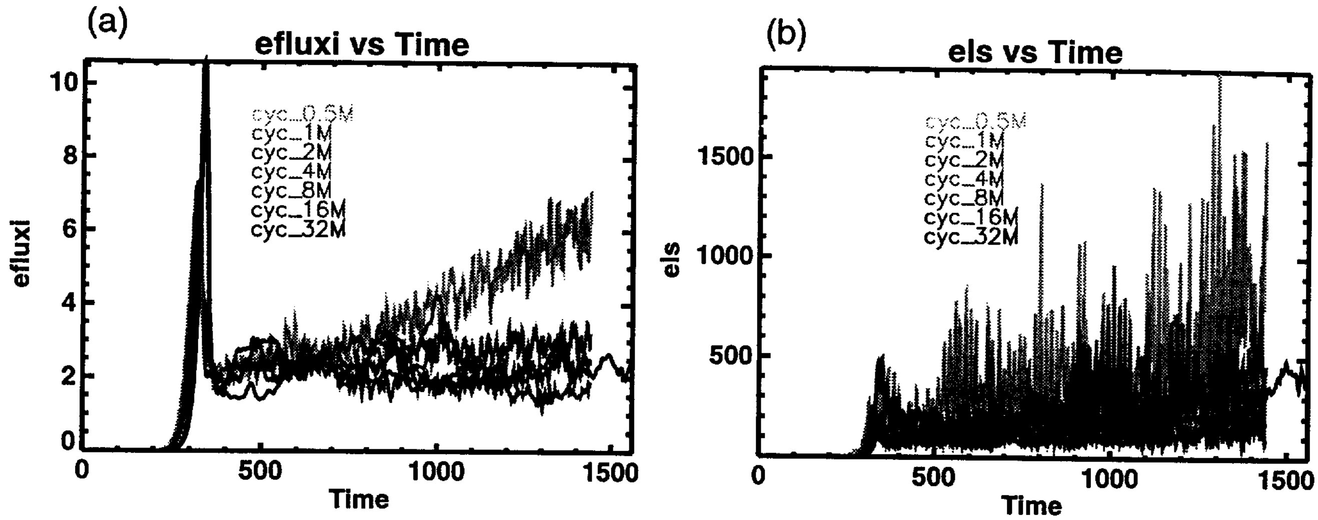

Figure 1. Particle-number can for cyclone DIII-D base case; (a) ion thermal diffusivity, (b) mean squared potential.

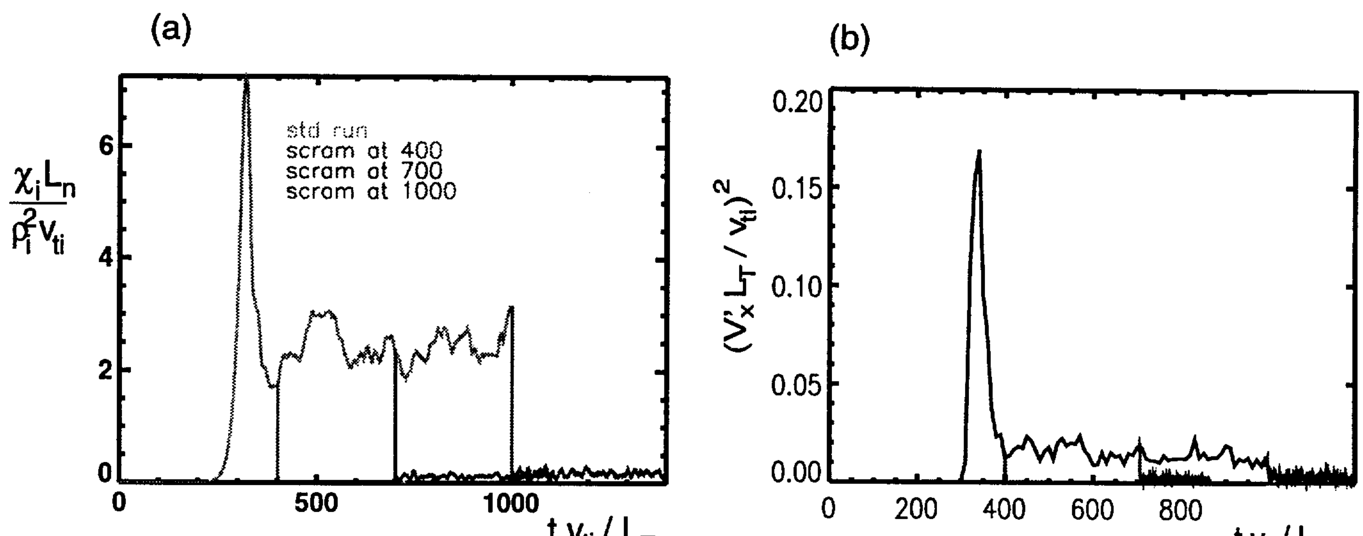

Figure 2. (a) Ion thermal diffusivity and (b) mean squared shearing rate from scrambling test.